ParFlow

Modeling Subsurface Flow and Chemical Migration on High Performance Computers

University of California
Lawrence Livermore National Laboratory

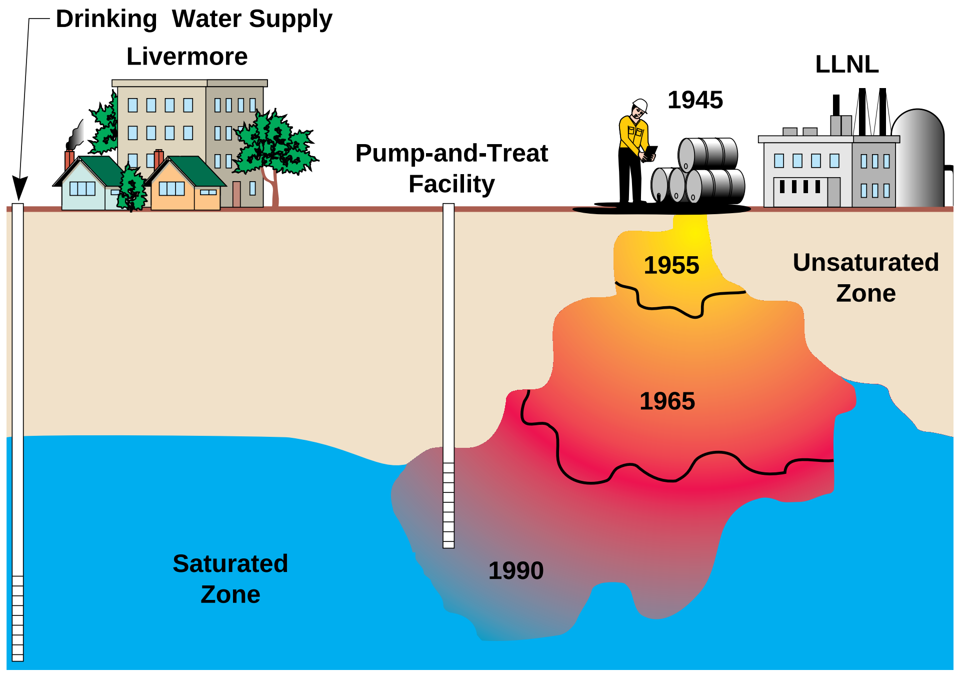
CASC Center for Applied Scientific Computing

Technology

The Center for Applied Scientific Computing at Lawrence Livermore National Laboratory has developed ParFlow, a subsurface flow simulation code. Parflow employs state-of-the-art computational methods and high-performance computing technology to enable detailed simulations of fluid flow and chemical transport in three-dimensional, heterogeneous porous media.

Applications

We are using ParFlow to design, manage, and evaluate groundwater remediation and water resource management strategies. Specifically, ParFlow is being used to study the efficacy of pump-and-treat remediation schemes, and to help municipalities manage their water supplies more efficiently.



Contaminants have migrated through the unsaturated zone into the more mobile groundwaters. LLNL is designing and implementing remediation procedures.

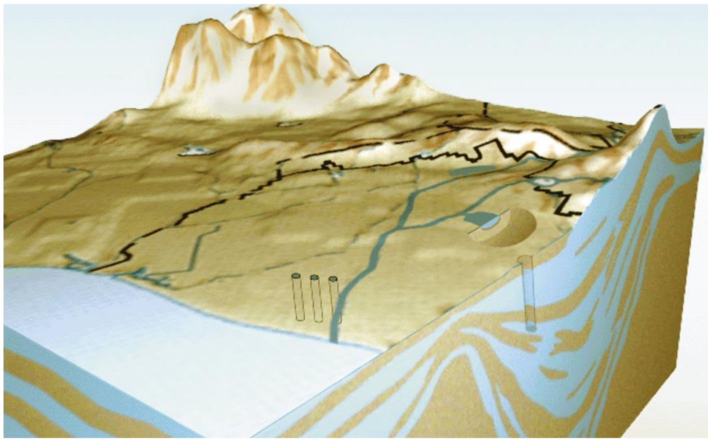
Groundwater remediation and water resource management are major environmental issues throughout the world. In the United States, for instance, numerous governmental and industrial sites, including Lawrence Livermore National Laboratory (LLNL), require remediation. At LLNL, chemical waste products were dumped onto the ground surface in the 1940s when the present site was a naval air station. LLNL is obligated to characterize the contamination and clean it up. Toward this end, various engineered remediation techniques are now being studied, tested, and implemented. Ground-water resource management is a related application of increasing importance, both domestically and internationally. The lack of adequate water supplies of sufficient quality is an impediment to growth in Southern California and a regional security issue in the Mideast.

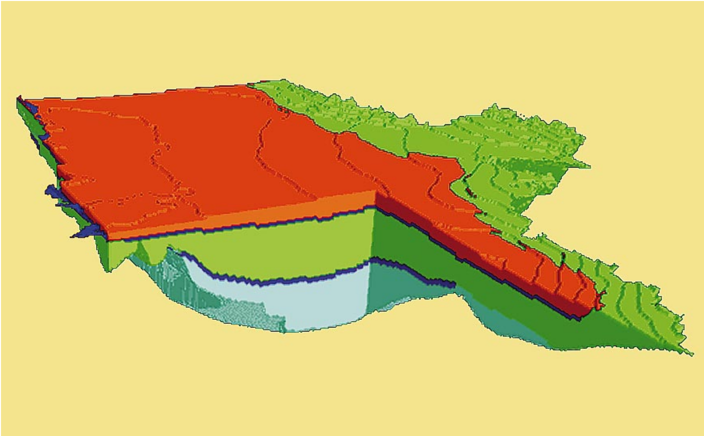
Numerical simulations can be used to determine the most cost-effective cleanup strategy for a contaminated site, as well as to study regional aquifer management issues. Unfortunately, the data required to accurately describe the structure and material characteristics of a subsurface formation, as well as the contaminant distribution within it, are usually not available because of the high cost of data acquisition and the impossibility of making measurements at all possible locations of interest. In addition, due to the nonuniform nature of the system, the quantitative distribution of properties, such as the hydraulic conductivity or reactive mineral abundance, can be quite variable. The sparsity and variation of the data can introduce a large element of uncertainty into modeling analyses. In order to compensate for these uncertainties, site managers typically over-engineer the remediation process, which increases costs.

To address this need for a more powerful simulation tool, we have developed ParFlow, a sophisticated software package for modeling fluid flow and chemical transport through heterogeneous porous media. To enable detailed simulations of real field sites, ParFlow uses state-of-the-art numerical methods and high-performance computing technologies. These simulations provide site managers with a more realistic picture of contaminant migration, thereby enabling a more cost-effective cleanup strategy. ParFlow also enables large-scale modeling of regional aquifers that encompass hundreds of square miles.

Enabling Large-Scale Simulations

The ParFlow simulator is being used to study groundwater flow and contaminant migration at several sites. The size of these sites (usually





ParFlow has been used to study water resource management issues for the Orange County Water District. An artist's depiction of the Orange County basin is shown on the left; our scalable conceptual model of the area to be modeled is shown on the right.

several square kilometers) and the need to resolve the subsurface heterogeneities (to within a few meters) result in grids with upwards of 100 million spatial zones; similarly sized problems arise in regional aquifer management studies. Since our researchers never have this much hard data about the composition of subsurface materials, we employ geostatistical techniques to generate statistically accurate subsurface realizations from the given field data. This is done in a fully parallel way, starting with a scalable conceptual model of the subsurface (which is defined with the help of the Army's versatile GMS package).

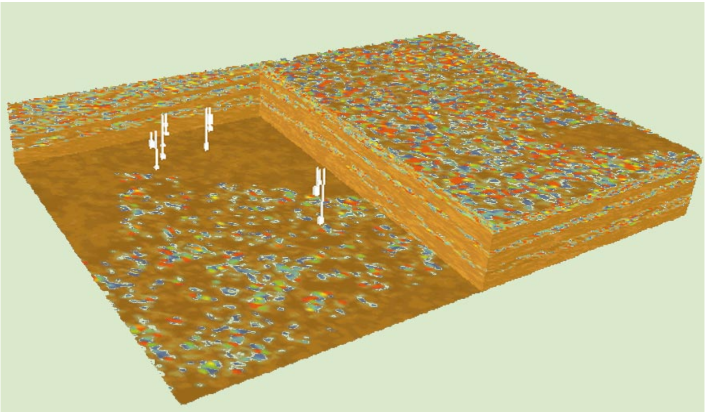
The modeling equations are discretized via finite volumes, and the resulting linear system is solved with a scalable multigrid-preconditioned conjugate gradient algorithm. The resulting flow velocity field is then passed to an advection code to simulate contaminant migration. We have a fully integrated and parallel grid-based Godunov method as our transport algorithm.

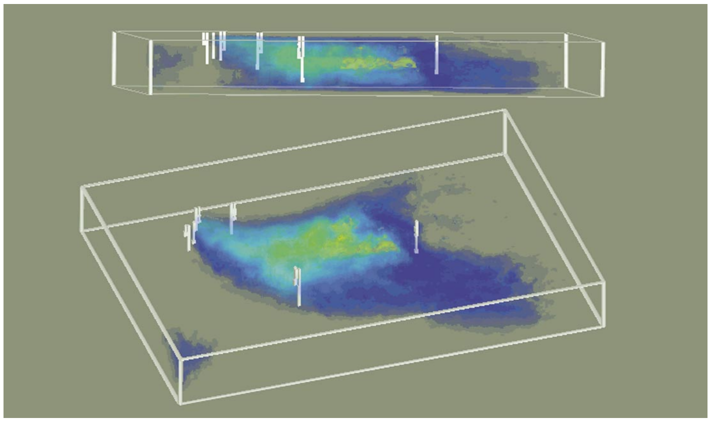
ParFlow is portable across a variety of computing platforms, ranging from workstations to massively parallel computers. Large simulations have been run on the Laboratory's IBM SP-2 and DEC Alpha cluster, as well as on the Intel ASCI red machine and on Cray T3D and T3E machines. We have demonstrated scalability on several MPP platforms, which means that our code makes efficient use of the additional processors needed for bigger simulations. Our flow solver is especially fast solving realistic flow problems involving eight million spatial zones in just 13 seconds on a 256-processor Cray T3D.

Multidisciplinary Collaboration

The ParFlow project is a multidisciplinary effort involving scientists from the Center for Applied Scientific Computing and Environmental Programs.

For additional information about the ParFlow project, contact Andrew Tompson, (925) 422-6348, tompson1@llnl.gov.





In collaboration with IT Corporation, we have used ParFlow to study various pump-and-treat remediation scenarios for a large industrial site in Northern California. Our scalable conceptual model of the heterogeneous subsurface (with screened pumping wells) is shown on the left. A snapshot in time of a simulation of plume migration is shown on the right.

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